wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 06:38 AM EDT

PDB ID	:	2ZV3
Title	:	Crystal structure of project MJ0051 from Methanocaldococcus jannaschii DSM 2661
Authors	:	Shimizu, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2008-10-31
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

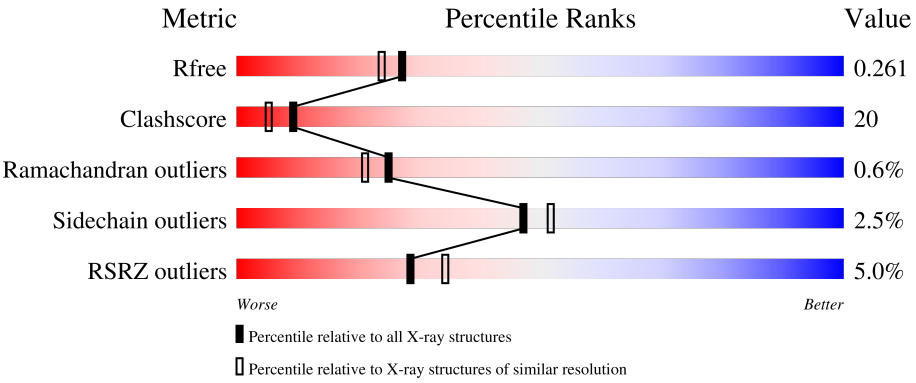
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



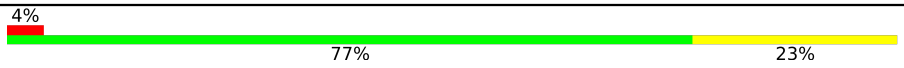
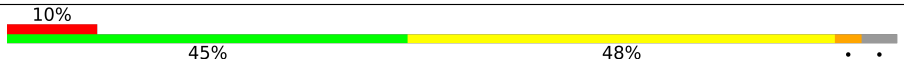
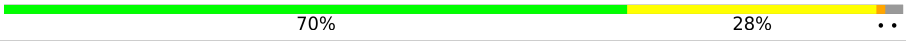
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	76% 18% 6%
1	B	115	3% 80% 19%
1	C	115	2% 73% 23%
1	D	115	2% 68% 31%
1	E	115	2% 72% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	115	
1	G	115	
1	H	115	
1	I	115	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8466 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-tRNA hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			833	525	151	152	5			
1	B	115	Total	C	N	O	S	0	0	0
			887	558	161	163	5			
1	C	111	Total	C	N	O	S	0	0	0
			854	538	156	155	5			
1	D	115	Total	C	N	O	S	0	0	0
			887	558	161	163	5			
1	E	115	Total	C	N	O	S	0	0	0
			887	558	161	163	5			
1	F	115	Total	C	N	O	S	0	0	0
			887	558	161	163	5			
1	G	110	Total	C	N	O	S	0	0	0
			844	532	153	154	5			
1	H	103	Total	C	N	O	S	0	0	0
			786	496	142	143	5			
1	I	113	Total	C	N	O	S	0	0	0
			870	548	157	160	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total	O	0	0
			101	101		
2	B	93	Total	O	0	0
			93	93		
2	C	87	Total	O	0	0
			87	87		
2	D	80	Total	O	0	0
			80	80		
2	E	80	Total	O	0	0
			80	80		

Continued on next page...

Continued from previous page...

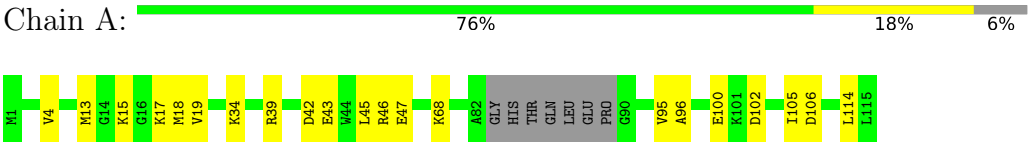
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	90	Total O 90 90	0	0
2	G	57	Total O 57 57	0	0
2	H	57	Total O 57 57	0	0
2	I	86	Total O 86 86	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

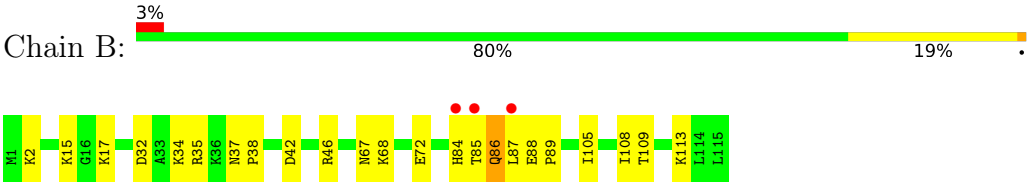
• Molecule 1: Peptidyl-tRNA hydrolase

Chain A:



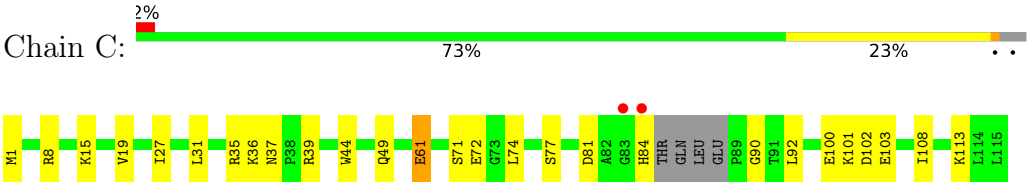
• Molecule 1: Peptidyl-tRNA hydrolase

Chain B:



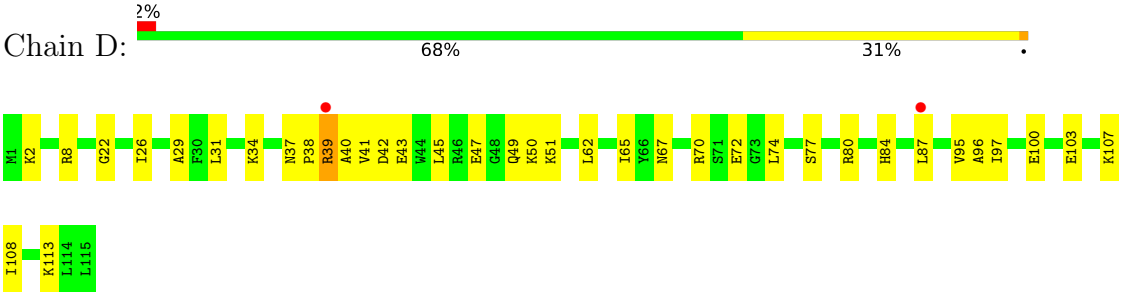
• Molecule 1: Peptidyl-tRNA hydrolase

Chain C:



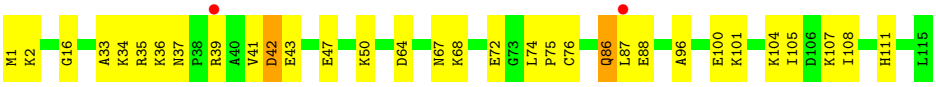
• Molecule 1: Peptidyl-tRNA hydrolase

Chain D:

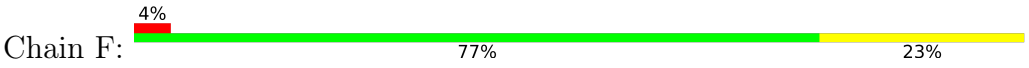


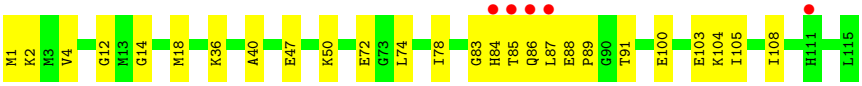
• Molecule 1: Peptidyl-tRNA hydrolase

Chain E:

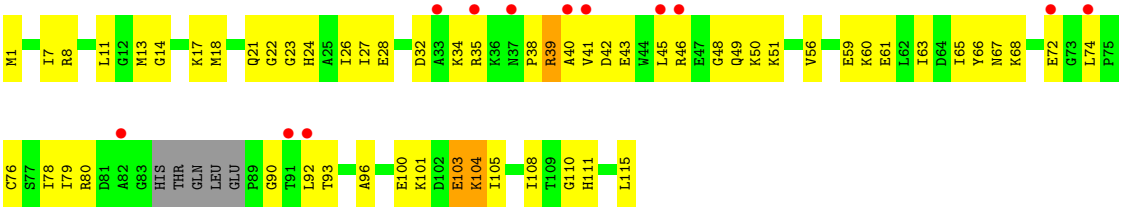


• Molecule 1: Peptidyl-tRNA hydrolase

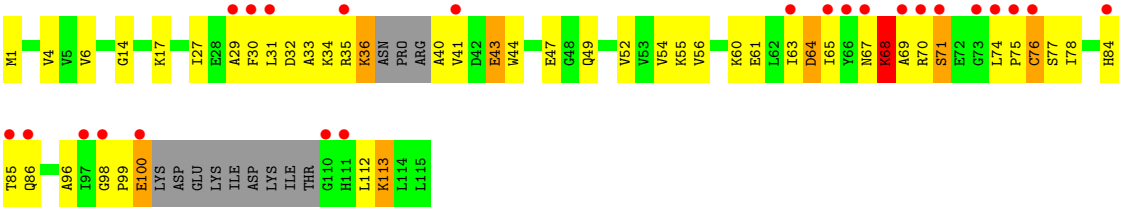




• Molecule 1: Peptidyl-tRNA hydrolase



• Molecule 1: Peptidyl-tRNA hydrolase



• Molecule 1: Peptidyl-tRNA hydrolase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.85Å 70.79Å 96.01Å 90.00° 121.67° 90.00°	Depositor
Resolution (Å)	40.92 – 2.10 40.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.92-2.10) 99.7 (40.92-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.263 0.217 , 0.261	Depositor DCC
R_{free} test set	2496 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/840	0.62	0/1120
1	B	0.39	0/897	0.62	0/1200
1	C	0.36	0/863	0.63	0/1151
1	D	0.37	0/897	0.67	0/1200
1	E	0.33	0/897	0.61	0/1200
1	F	0.36	0/897	0.62	0/1200
1	G	0.38	0/852	0.61	0/1136
1	H	0.52	0/793	0.84	1/1058 (0.1%)
1	I	0.37	0/878	0.62	0/1172
All	All	0.39	0/7814	0.65	1/10437 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	68	LYS	O-C-N	5.70	131.81	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	76	CYS	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	833	0	891	22	0
1	B	887	0	941	23	0
1	C	854	0	909	20	0
1	D	887	0	941	33	0
1	E	887	0	941	31	0
1	F	887	0	941	33	0
1	G	844	0	902	67	0
1	H	786	0	831	84	0
1	I	870	0	926	27	1
2	A	101	0	0	4	0
2	B	93	0	0	5	0
2	C	87	0	0	8	0
2	D	80	0	0	5	0
2	E	80	0	0	7	0
2	F	90	0	0	7	0
2	G	57	0	0	3	0
2	H	57	0	0	7	0
2	I	86	0	0	4	0
All	All	8466	0	8223	316	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 316 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ALA:HB1	1:H:41:VAL:HG21	1.26	1.14
1:H:14:GLY:H	1:H:17:LYS:HD2	1.03	1.13
1:D:2:LYS:HB3	1:D:50:LYS:HE3	1.42	1.01
1:H:14:GLY:N	1:H:17:LYS:HD2	1.80	0.96
1:F:88:GLU:HG3	1:F:89:PRO:HD2	1.49	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:LYS:NZ	1:I:34:LYS:NZ[2_556]	1.89	0.31

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	104/115 (90%)	104 (100%)	0	0	100 100
1	B	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	17 12
1	C	107/115 (93%)	101 (94%)	6 (6%)	0	100 100
1	D	113/115 (98%)	109 (96%)	4 (4%)	0	100 100
1	E	113/115 (98%)	110 (97%)	3 (3%)	0	100 100
1	F	113/115 (98%)	111 (98%)	2 (2%)	0	100 100
1	G	106/115 (92%)	101 (95%)	3 (3%)	2 (2%)	8 3
1	H	97/115 (84%)	84 (87%)	10 (10%)	3 (3%)	4 1
1	I	109/115 (95%)	107 (98%)	2 (2%)	0	100 100
All	All	975/1035 (94%)	935 (96%)	34 (4%)	6 (1%)	25 21

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	GLN
1	H	68	LYS
1	H	70	ARG
1	H	71	SER
1	G	110	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/95 (94%)	87 (98%)	2 (2%)	52	57
1	B	95/95 (100%)	93 (98%)	2 (2%)	53	59
1	C	91/95 (96%)	89 (98%)	2 (2%)	52	57
1	D	95/95 (100%)	94 (99%)	1 (1%)	73	79
1	E	95/95 (100%)	92 (97%)	3 (3%)	39	41
1	F	95/95 (100%)	94 (99%)	1 (1%)	73	79
1	G	90/95 (95%)	87 (97%)	3 (3%)	38	40
1	H	83/95 (87%)	77 (93%)	6 (7%)	14	11
1	I	93/95 (98%)	92 (99%)	1 (1%)	73	79
All	All	826/855 (97%)	805 (98%)	21 (2%)	47	52

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	36	LYS
1	H	68	LYS
1	I	101	LYS
1	H	100	GLU
1	H	64	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	86	GLN
1	E	111	HIS
1	I	67	ASN
1	H	84	HIS
1	I	57	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	108/115 (93%)	-0.53	0 100 100	7, 17, 27, 41	0
1	B	115/115 (100%)	-0.17	3 (2%) 56 61	12, 22, 41, 62	0
1	C	111/115 (96%)	-0.23	2 (1%) 68 72	14, 25, 46, 58	0
1	D	115/115 (100%)	0.01	2 (1%) 70 74	13, 29, 54, 66	0
1	E	115/115 (100%)	-0.01	2 (1%) 70 74	15, 28, 51, 56	0
1	F	115/115 (100%)	-0.04	5 (4%) 35 41	13, 27, 52, 73	0
1	G	110/115 (95%)	0.74	12 (10%) 5 7	20, 43, 81, 85	0
1	H	103/115 (89%)	1.14	24 (23%) 0 0	20, 44, 68, 75	0
1	I	113/115 (98%)	-0.12	0 100 100	11, 27, 50, 55	0
All	All	1005/1035 (97%)	0.08	50 (4%) 28 34	7, 28, 58, 85	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	74	LEU	8.6
1	H	41	VAL	5.9
1	F	86	GLN	4.7
1	H	97	ILE	4.6
1	H	65	ILE	4.6

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.